इंडियन इंस्टीट्यूट ऑफ टेक्नोलॉजी दिल्ली

हौज खास, नई दिल्ली -110016

(औद्योगिक अनुसंधान एवं विकास इकाई)

INDIAN INSTITUTE OF TECHNOLOGY DELHI

Hauz Khas, New Delhi-110016

(Industrial Research & Development Unit)

No. IITD/IRD/MI00148/ 363998

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Applications from Indian nationals, Persons of Indian Origin (PIOs), and Overseas Citizens of India (OCIs) for the Post-Doctoral Fellows (PDF) at Multiphysics and Multiscale Research Group (M3RG), Department of Civil Engineering are invited for Project Appointment under the following project. Appointment shall be on contractual basis with consolidated pay, renewable yearly or upto the duration of the project, whichever is earlier.

Project Summary: Oxide glasses form a major part of our daily lives, starting from cell phone screens, window glasses, optical fibers (that are used for delivering high-speed internet), to the bio-glasses used in medical applications, and high-level waste glass (used for immobilization of nuclear waste). However, glass being a non-crystalline solid is quite challenging to model when it comes to atomistic simulations. This has led to a dearth of suitable interatomic potentials, which limits its wider applicability. Here, we propose a machine learning (ML) based approach to develop the novel interatomic potential for simulating oxide glasses. The ML potential, namely, Python for Glass Genomics Force Field (PyGGi-FF), will use the data from ab-initio simulations to develop novel potentials based on the topology of the atomic structure. Specifically, we will employ graph networks that can learn the interactions between atomic systems to model the interactions between different atoms. Further, symbolic regression will be employed on the models to develop empirical forms for the potentials. These potentials will finally be incorporated in widely used open-source packages such as LAMMPS for the wider applicability of the developed potential. All the potentials developed will be made available publicly as part of the PyGGi package (see: http://pyggi.iitd.ac.in). In summary, this project proposes developing a scalable and transferable machine learned interatomic potential repository for oxide glasses that can enable accelerated high-throughput simulations and insights into the fundamental behavior of materials.

Title of the Project	Professional Development Fund of Prof. Anoopkrishnan Naduvath Mana (16748)	
Funding Agency	IRD Unit, IIT DELHI	
Name of the Project Investigator	Prof. Anoopkrishnan Naduvath Mana [email ID: krishnan@iitd.ac.in]	
Deptt/.Centre	Department of Civil Engineering / School of Artificial Intelligence	
Duration of the Project	Upto:03/05/2030	
Post (s)	Consolidated fellowship / Pay-slab	Qualifications
Principal Project Scientist (1)	Rs.56,000-60,000-64,000-69,000-74,000-79,000/- p.m. (consolidated)	1. Ph.D. degree with research background and HPC experience in molecular modelling (chemistry/physics/chemical/materials/bio), bioinformatics and computational biology, atmospheric/oceanic sciences, AI/ML, CFD, etc. 2. Maximum age is 32 years for males and 35 years for female candidates (to be relaxed by 5 years in case of persons with physical disability, SC and ST, and 3 years in case of OBC-NCL). 3. At least 2 referred conference/journal papers (of which at least 1 should be in scopus journal

The candidates who are interested to apply for the above post should download **Form No. IRD/REC-4** from the IRD Website (http://ird.iitd.ac.in/rec) of IIT Delhi and submit the duly filled form with complete information regarding educational qualifications indicating percentage of marks/division, details of work experience etc. **by e-mail with advertisement No. on the subject line to Prof. Anoopkrishnan Naduvath Mana at email id: krishnan@iitd.ac.in**

IIT Delhi reserves the right to fix higher criteria for short-listing of eligible candidates from those satisfying advertised qualification and requirement of the project post and their name will be displayed on web link (http://ird.iitd.ac.in/shortlisted) alongwith **the online interview details. Only short-listed candidates will be informed for online interview**. In case any clarification is required on eligibility regarding the above post, the candidate may contact **Prof. Anoopkrishnan Naduvath Mana at email id: krishnan@iitd.ac.in**

5% relaxation of marks may be granted to the SC/ST Candidates. In case of selection of a retired/superannuated government employee, his/her salary will be fixed as per prevailing IRD norms. अनुसूचित जाति / अनुसूचित जनजाति के उम्मीदवारों को अंकों की 5% छूट दी जा सकती है. एक सेवानिवृत्त सरकारी कर्मचारी के चयन के मामले में उसका वेतन वर्तमान आईआरडी मानदंडों के अनुसार तय किया जाएगा। **The last date for submitting the completed applications by e-mail is 05/11/2021 by 5.00 p.m.**

सहायक कुलसचिव, आईआरडी

वितरण

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